A NEW EQUATION OF STATE FOR SOLID $para$-HYDROGEN

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Solid *para*-H_2 is a popular accommodating host for impurity spectroscopy due to its unique softness and the spherical symmetry of *para*-H_2 in its J=0 rotational level.[a,b] To simulate the properties of impurity-doped solid *para*-H_2, a reliable model for the 'soft' pure solid *para*-H_2 at different pressures is highly desirable. While a couple of experimental[c] and theoretical[d] studies aimed at elucidating the equation of state (EOS) of solid *para*-H_2 have been reported, the calculated EOS was shown to be heavily dependent on the potential energy surface (PES) between two *para*-H_2 that was used in the simulations.[e] The current study also demonstrates that different choices of the parameters governing the Quantum Monte Carlo simulation could produce different EOS curves.

To obtain a reliable model for pure solid *para*-H_2, we used a new 1-D *para*-H_2 PES reported by Faruk *et al.*[f] that was obtained by averaging over Hinde's highly accurate 6-D H_2–H_2 PES.[g] The EOS of pure solid *para*-H_2 was calculated using the PIMC algorithm with periodic boundary conditions (PBC). To precisely determine the equilibrium density of solid *para*-H_2, both the value of the PIMC time step τ and the number of particles in the PBC cell were extrapolated to convergence. The resulting EOS agreed well with experimental observations, and the *hcp* structured solid *para*-H_2 was found to be more stable than the *fcc* one at 4.2K, in agreement with experiment. The vibrational frequency shift of *para*-H_2 as a function of the density of the pure solid was also calculated, and the value of the shift at the equilibrium density is found to agree well with experiment.

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